Monday 23 June

Session A1 – 8:30		**Session B1**		**Session C1**		**Session D1**		**Session E1**	
CATALYSIS & REACTIVITY		ELECTRONIC-STRUCTURE THEORY		BIOSYSTEMS		COMPUTING & SOFTWARE		CHEMICAL STRUCTURE & BONDING	
Reactants, reactions, and catalysis		Green's function methods		Cheminform. & medicinal chemistry		Quantum computing		Conjugated systems	
Kevin Naidoo		*Andreas Görling*		*Stacey Wetmore*		*Ivan Kassal*		*Peter Schreiner*	
Raghavan Sunoj	963	Dominika Zgid	924	Jean-Louis Reymond	986	Birgitta Whaley	919	Debashree Ghosh	871
Stuart Macgregor	926	Wim Klopper	458	Jan Řezáč	480	Artur Izmaylov	131	Abhik Ghosh	973
Ashique Lal	207	Marios-Petros Kitsaras	124	Elfi Kraka	130	Davide Castaldo	327	Martin Rahm	23
Boris Maryasin	127	Arno Förster	572	Jean-Philip Piquemal	699	Karl Michael Ziems	260	Takafumi Shiraogawa	313
Session A2 - 10:20		**Session B2**		**Session C2**		**Session D2**		**Session E2**	
MACHINE LEARNING		CATALYSIS & REACTIVITY		ELECTRONIC-STRUCTURE THEORY		BIOSYSTEMS		ELECTRONIC-STRUCTURE THEORY	
ML for simulations		Surfaces and heterogenous catalysis		Numerical methods and techniques		Macromolecules		Ultrahigh accuracy and QED	
Heather Kulik		*Angel Martín Pendás*		*Stefan Grimme*		*Benedetta Mennucci*		*Fritz Schaefer*	
Gábor Csányi	967	Philippe Sautet	873	Peter Gill	953	Lynn Kamerlin	49	Trond Saue	349
Alexandre Tkatchenko	995	Núria López	972	Luca Frediani	896	Subha Kalyaanamoorthy	653	Jacek Komasa	178
Jelle Vekeman	785	Christopher Stein	287	Alexander Stark	157	Xiang Sheng	196	Ádám Margócsy	775
Michael Gillhofer	317	Mireia Segado-Centellas	716	Eduard Matito	136	Adil Kabylda	547	Pekka Pyykkö	486
Session A3 – 13:20		**Session B3**		**Session C3**		**Session D3**		**Session E3**	
ELECTRONIC-STRUCTURE THEORY		ENERGY & MATERIALS		CATALYSIS & REACTIVITY		QUANTUM DYNAMICS		BIOSYSTEMS	
Coupled-cluster theory		Condensed systems		Molecular and reaction design		Nonadiabatic dynamics		Macromolecules	
Jürgen Gauss		*Yi Qin Gao*		*Vidar Remi Jensen*		*Ove Christiansen*		*Elfi Kraka*	
Piotr Piecuch	923	Francesco Paesani	752	Yousung Jung	441	Alicia Palacios	804	Ferran Feixas	622
Henrik Koch	862	Damien Laage	918	Jan H. Jensen	440	Jian Liu	86	Taye Demissie	673
Karol Kowalski	199	Jochen Blumberger	54	Kevin Naidoo	171	Peter Schürger	166	Petra Imhof	339
Francesco Evangelista	348	Marco Nascimento	223	Gyula Hoffka	815	Oliver Kühn	412	Ana Gamiz-Hernandez	917
Session A4 – 15:10		**Session B4**		**Session C4**		**Session D4**		**Session E4**	
ELECTRONIC-STRUCTURE THEORY		MACHINE LEARNING		BIOSYSTEMS		CHEMICAL STRUCTURE & BONDING		QUANTUM DYNAMICS	
Explicit correlation		ML for chemical reactions		Macromolecules		Early elements		Ultrafast dynamics	
Wim Klopper		*Sigbjørn Løland Bore*		*Qiang Cui*		*Gabriel Merino*		*Thomas Bondo Pedersen*	
Seiichiro Ten-no	874	Boris Kozinsky	971	Modesto Orozco	819	Miroslav Urban	270	Francçise Remacle	887
Ali Alavi	853	Fernanda Duarte	842	Alessandra Magistrato	202	ED Jemmis	163	Michal Repisky	962
Éva Zsuzsanna Mihálka	470	Joakim Jestilä	246	Mariastella Cascone	544	Celina Sikorska	738	H. Bernhard Schlegel	197
Silvia di Grande	587	Jessica White	667	David Carrasco De Busturia	165	Tatiana Korona	276	Jonathan Fetherolf	701
Session A5 – 17:00		**Session B5**		**Session C5**		**Session D5**		**Session E5**	
ELECTRONIC-STRUCTURE THEORY		MACHINE LEARNING		COMPUTING & SOFTWARE		QUANTUM DYNAMICS		CATALYSIS & REACTIVITY	
Density-functional development		ML for chemical design		Quantum computing		Ultrafast dynamics		Electrochemistry and related	
Weitao Yang		*David Balcells*		*Birgitta Whaley*		*Federica Agostini*		*Cristina Trujillo*	
Martin Head-Gordon	957	Clémence Corminbœuf	446	Ivan Kassal	356	Fernando Martín García	663	Samira Siahrostami	21
Erin Johnson	505	Anatole von Lilienfeld	442	Marco Govoni	902	Ove Christiansen	959	Maria Besora	402
Fritz Schaefer	687	Konstantinos Vogiatzis	10	Maria-Andreea Filip	419	Jiří Vaníček	691	Tangui Le Bahers	169
Viktor Staroverov	154	Thijs Stuyver	43	Yu Zhang	20	Nazanin Jamshidi	140	Melissa Manetsch	362

Tuesday 24 June

Session A1 – 8:30		**Session B1**		**Session C1**		**Session D1**		**Session E1**	
CATALYSIS & REACTIVITY		ELECTRONIC-STRUCTURE THEORY		BIOSYSTEMS		ELECTRONIC-STRUCTURE THEORY		SPECTROSCOPY	
Surfaces and heterogenous catalysis		Many-body methods & NCI		Bio/nanosystems		Relativistic quantum chemistry		Polarization models	
Stuart Macgregor		*Seiichiro Ten-no*		*Michele Cascella*		*Trond Saue*		*Russell Boyd*	
Anastassia Alexandrova	38	Katarzyna Pernal	875	Daan Frenkel	703	Wenjian Liu	436	Benjamin Stamm	798
Ataualpa Braga	901	Janus Juul Eriksen	810	Wataru Shinoda	782	Jürgen Gauss	438	Kaline Coutinho	938
Mikhail Polynski	357	Daniel Boese	443	Katie Wilson	97	Achintya Kumar Dutta	215	Cedrix Dongmo Foumthuim	624
Basil Raju	47	Andreas Hansen	121	João Coimbra	597	Erik Donovan Hedegård	497	Tommaso Nottoli	305
Session A2 - 10:20		**Session B2**		**Session C2**		**Session D2**		**Session E2**	
CATALYSIS & REACTIVITY		ENERGY & MATERIALS		ELECTRONIC-STRUCTURE THEORY		QUANTUM DYNAMICS		BIOSYSTEMS	
Molecular and reaction design		Materials and energy		Berry phase & complex wavefunctions		Ultrafast dynamics		Bio/nanosystems	
Odile Eisenstein		*Leticia González*		*Henrik Koch*		*Fernando Martín García*		*Modesto Orozco*	
Satoshi Maeda	307	Laura Gagliardi	702	Hardy Gross	949	Federica Agostini	388	Biswarup Pathak	921
Markus Reiher	80	Elena Besley	763	Joseph Subotnik	686	Morgane Vacher	820	Matteo Dal Peraro	728
Derek Ahneman	161	Tim Kowalczyk	239	Ansgar Pausch	581	Yi Zhao	720	Gioacchino Schifino	580
Giovannimaria Piccini	698	Shubhajit Das	609	Bang Huynh	191	Angela Wilson	680	Samaneh Davoudi	79
Session A3 – 13:20		**Session B3**		**Session C3**		**Session D3**		**Session E3**	
ELECTRONIC-STRUCTURE THEORY		MACHINE LEARNING		BIOSYSTEMS		QUANTUM DYNAMICS		CHEMICAL STRUCTURE & BONDING	
Density-functional development		ML for chemical reactions		Cheminform. & medicinal chemistry		DMRG and MCTDH		f-block elements	
Miroslav Urban		*Francesco Paesani*		*Ursula Röthlisberger*		*Françoise Remacle*		*Pekka Pyykkö*	
Kieron Burke	922	Teresa Head-Gordon	847	William Jorgensen	808	Irene Burghardt	666	Karin Fink	722
Eunji Sim	807	Dennis Salahub	91	Zoe Cournia	981	Zhigang Shuai	773	Miho Hatanaka	713
Jacques Desmarais	128	Jordi Buils	479	Stacey Wetmore	321	Yuki Kurashige	56	Sergey Varganov	524
Priya Priya	692	Haobo Li	26	Christoph Riplinger	714	Henrik Larsson	134	Meagan Oakley	700
Session A4 – 15:10		**Session B4**		**Session C4**		**Session D4**		**Session E4**	
CATALYSIS & REACTIVITY		SPECTROSCOPY		BIOSYSTEMS		ELECTRONIC-STRUCTURE THEORY		ENERGY & MATERIALS	
Surfaces and heterogenous catalysis		Methods for excited electronic states		Multiscale modelling		Strong correlation & entanglement		Condensed systems	
Raghavan Sunoj		*Frank Neese*		*Marco De Vivo*		*Gustavo Scuseria*		*Marco Nascimento*	
Annabella Selloni	748	Emmanuel Fromager	755	Benedetta Mennucci	832	Shuhua Li	881	Nicola Gaston	955
Akira Nakayama	681	Weitao Yang	956	Paula Homem-de-Mello	685	Mario Piris	16	Pavel Jungwirth	664
Seungjae Kwak	437	Momir Mališ	787	Yingjie Wang	117	Jiří Pittner	77	Sheh-Yi Sheu	19
Francesc Viñes Solana	89	Lars Goerigk	139	Sebastian Reiter	594	Sarai Dery Folkestad	94	Jun-Ho Choi	50
Session A5 – 17:00		**Session B5**		**Session C5**		**Session D5**		**Session E5**	
MOLECULAR DYNAMICS		ELECTRONIC-STRUCTURE THEORY		CATALYSIS & REACTIVITY		SPECTROSCOPY		EXOTIC SYSTEMS	
Honorary session: 40 years of AIMD		Methods for larger systems		Reactants, reactions, and catalysis		Circular dichroism		Strong fields and high pressure	
Matteo Dal Peraro		*David Sherrill*		*Annia Galano*		*Kenneth Ruud*		*Peter Schwerdtfeger*	
Roberto Car	987	Christian Ochsenfeld	952	David Wales	969	Daniel Crawford	757	Stella Stopkowicz	941
Ursula Röthlisberger	960	Hiromi Nakai	723	Feliu Maseras	674	Luuk Visscher	814	Andrew Wibowo-Teale	671
Mark Tuckerman	395	Filippo Lipparini	826	Sebastian Kozuch	2	WanZhen Liang	243	Eva Zurek	697
Amin Alibakhshi	771	Maristella Alessio	187	Masataka Nagaoka	44	Marco Caricato	138	Mercedes Alonso	393

Thursday 26 June

Session A1 – 8:30		**Session B1**		**Session C1**		**Session D1**		**Session E1**	
ELECTRONIC-STRUCTURE THEORY		SPECTROSCOPY		BIOSYSTEMS		CHEMICAL STRUCTURE & BONDING		ENERGY & MATERIALS	
Methods for periodic systems		Methods for excited states		Multiscale modelling		Analysis		Photophysics and photochemistry	
Christian Ochsenfeld		*Emmanuel Fromager*		*Stefano Vanni*		*Henry Rzepa*		*Zhigang Shuai*	
Georg Kresse	831	Julia Westermayr	364	Qiang Cui	689	Matthias Bickelhaupt	670	Dage Sundholm	797
Lin Lin	571	Hannes Jońsson	660	Garnet Chan	872	Frank de Proft	813	Jin Wen	800
David Tew	870	Thomas Froitzheim	81	Andrea Pérez-Villa	504	Inbal Tuvi-Arad	749	Dana Nachtigallová	636
Philip Hoggan	13	Elli Selenius	790	Andrea Levy	601	Jacob Toney	394	Sofia Canola	582
Session A2 - 10:20		**Session B2**		**Session C2**		**Session D2**		**Session E2**	
ELECTRONIC-STRUCTURE THEORY		CATALYSIS & REACTIVITY		BIOSYSTEMS		ENERGY & MATERIALS		COMPUTING & SOFTWARE	
Simpler model systems		Reactants, reactions, and catalysis		Multiscale modelling		Photophysics and photochemistry		Software	
Anna Krylov		*Manuel Yañez*		*Garnet Chan*		*Dage Sundholm*		*Daniel Crawford*	
Stefan Grimme	825	Evert Jan Meijer	943	Carme Rovira	863	Kumar Vanka	899	Patrick Norman	898
Peter Schwerdtfeger	92	Bastian Skjelstad	715	Marco De Vivo	817	Leticia González	964	Susi Lehtola	799
Per Siegbahn	212	Amalia Poblador Bahamonde	880	Stefano Serapian	120	Enrico Tapavicza	523	John Herbert	24
Itai Panas	679	Zhexuan Song	654	Allison Keys	226	Enrique Manuel Arpa	411	David Sherrill	513
Session A3 – 13:20		**Session B3**		**Session C3**		**Session D3**		**Session E3**	
ELECTRONIC-STRUCTURE THEORY		CATALYSIS & REACTIVITY		MACHINE LEARNING		SPECTROSCOPY		TEACHING & EDUCATION	
Density-functional development		Molecular and reaction design		ML for simulations		Rotovibrational spectra		Teaching & education	
Jiali Gao		*Ainara Nova*		*Konstantinos Vogiatzis*		*Sonia Coriani*		*Trygve Helgaker*	
Stefan Vučković	837	Annia Galano	508	Yi Luo	737	Attila Császár	931	Anders Malthe-Sorenssen	998
Martin Kaupp	661	Vidar Remi Jensen	946	Yi Qin Gao	882	Guntram Rauhut	106	Peter Taylor	1001
Hans Jorgen Aa. Jensen	457	Cristina Trujillo	36	Amanda Arcidiacono	537	Ayaki Sunaga	735	Dirk Andrae	367
Aaron Garrison	159	Wataru Matsuoka	237	Krzysztof Szalewicz	730	Frederik Tielens	72	Henry Rzepa	12
Session A4 – 15:10		**Session B4**		**Session C4**		**Session D4**		**Session E4**	
CATALYSIS & REACTIVITY		ENERGY & MATERIALS		ELECTRONIC-STRUCTURE THEORY		MACHINE LEARNING		SPECTROSCOPY	
Reactants, reactions, and catalysis		Materials and energy		Optimization in quantum chemistry		ML for electronic structure		Positrons & weak interactions	
Feliu Maseras		*Evert Jan Meijer*		*Erik Tellgren*		*Hiromi Nakai*		*Edit Mátyus*	
Jing Ma	888	Debra Bernhardt	751	Éric Cances	742	Paola Gori-Giorgi	867	Gustavo Aucar	861
Fahmi Himo	928	Sara Bonella	827	Roland Lindh	672	Matthias Kick	233	Robert Berger	360
Johannes Hoja	575	Virginia Carnevali	538	Giovanni Scalmani	619	Angel Martín Pendás	58	Dermot Green	256
Michele Assante	769	Tuanan Lourenço	334	Hugh Burton	712	Tomáš Bučko	214	Kenneth Jordan	1
Session A5 – 17:00		**Session B5**		**Session C5**		**Session D5**		**Session E5**	
SPECTROSCOPY		ELECTRONIC-STRUCTURE THEORY		ENERGY & MATERIALS		BIOSYSTEMS		CHEMICAL STRUCTURE & BONDING	
Spectroscopy & energy surfaces		Beyond standard DFT		Materials and energy		Bio/nanosystems		Coordination chemistry	
Abril Castro		*Paola Gori-Giorgi*		*Laura Gagliardi*		*Carme Rovira*		*ED Jemmis*	
Sonia Coriani	925	Paul Ayers	733	Marie-Liesse Doublet	966	Sergio Pantano	417	Gabriel Merino	392
Anna Krylov	382	Jiali Gao	904	Emi Minamitani	93	Cristiana Di Valentin	794	Jeanet Conradie	118
Ida-Marie Høyvik	721	Andreas Görling	220	Gloria I. Cárdenas-Jirón	795	Stefano Vanni	643	Julien Panetier	53
Takeshi Sato	651	Lucien Dupuy	631	Antti Karttunen	607	Maurício Coutinho Neto	732	Konrad Patkowski	122